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New way of looking at the Brownian motion of two interacting particles

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Abstract : It is shown how to rewrite the underlying Fokker-Planck equation using step function for the Brownian motion of two interacting particles under a square well potential. This makes it much simpler to find the complete solution of the problem.

Keyword : Brownian motion problem

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The problem of Brownian motion and its generalisations have been of considerable interest to many physicists since the time when Einstein first calculated the mean square value of the displacement of a free particle. It is now well known that one has to solve the underlying partial differential equation called the Fokker-Planck equation to find the probability distribution function which can then be used to calculate the quantities of interest like the mean square displacement. The partial differential equation has to be solved with the given initial value and boundary conditions. Recently Morita [1] had solved the problem of Brownian motion of two interacting particles under a square well potential. Later Berdichevsky and Gitterman [2] had pointed out that the solution of the Brownian motion problem given by Morita cannot be correct as it does not give the Einstein's relation. The aim of the present work is to rewrite the partial differential equation using step function which shows that the equation for the Brownian motion in the present case is the same as the usual diffusion equation except at the point where the barrier is located. This form makes it extremely easy to calculate the discontinuities across the barrier.

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We follow the notation and the units of Berdichevsky and Gitterman [2] and write the Fokker-Planck equation for a particle escaping from the square well potential under the influence of white noise as

$$\partial_t \rho = \partial_x\left[\partial_x \rho + A\delta(x-u)\rho\right], \tag{1}$$

where V_0 is the depth of the potential well and u its width, $A = V_0/T$, the temperature T being measured in units of energy, while time is measured in units of length squared and the diffusion coefficient is taken as unity.

The initial condition for the probability distribution function ρ (x, t) is taken as

$$\rho(x,0) = \delta(x-u), \tag{2}$$

while the boundary conditions at $x = 0$ and $x = \infty$ are respectively :

$$\partial_x \rho = 0 \text{ and } \rho \text{ finite.} \tag{3}$$

Using the step function $\theta(v)$,

$$\theta(v) = 1 \quad \text{if } v > 1, \tag{4a}$$

$$\theta(v) = 0 \quad \text{if } v < 0, \tag{4b}$$

we can rewrite equation (1) as

$$\partial_t \rho = \partial_x\left\{\exp[A\theta(u-x)]\, \partial_x\left[\exp[-A\theta(u-x)]\rho\right]\right\}. \tag{5}$$

From eq. (5) we see that for both the regions $x < u$ as well as $x > u$, ρ (x, t) satisfies the usual one-dimensional diffusion equation

$$\frac{\partial \rho(x,t)}{\partial t} \qquad \frac{\partial^2 \rho(x,t)}{\partial x^2} \tag{6}$$

This is also the same partial differential equation which one encounters in the heat conduction problem [3]. To take into account the initial condition given by (2), one uses the Laplace transform $\hat{\rho}(x,s)$ defined by [3]

$$\hat{\rho}(x,s) = \int_0^\infty \exp(-st)\rho(x,t). \tag{7}$$

Using equations (2), (6) and (7) we find that the differential equation satisfied by $\hat{\rho}(x,s)$ for both $x < u$ as well as $x > u$ is

$$\frac{\partial^2 \hat{\rho}(x,s)}{\partial x^2} = s\hat{\rho}(x,s). \tag{8}$$

The two linearly independent solutions of eq. (8) are $\exp(\pm\sqrt{s}x)$ Using the boundary conditions (3), we find that the solution in the two regions is given by

$$\hat{\rho}_1(x,s) = C_1 \cosh\left(\sqrt{s}x\right) \quad 0 < x < u, \tag{9a}$$

$$\hat{\rho}_2(x,s) = C_2 \exp\left(-\sqrt{s}x\right) \quad u < x < \infty, \tag{9b}$$

The constants C_1, C_2 are determined by calculating the discontinuities in the values of $\rho(x, t)$ and its derivative across the boundary $x = u$.

We show the explicit calculation for the derivative using our eq. (5). Integrating eq. (5) from $x = u - \varepsilon$ to $x = u + \varepsilon$, $\varepsilon \to 0$, and using the property of the step function

$$\frac{\partial}{\partial t} \int_{x=u-\varepsilon}^{u+\varepsilon} \rho(x,t)dx = \left.\frac{\partial \rho(x,t)}{\partial x}\right|_{u+\varepsilon} - \left.\frac{\partial \rho(x,t)}{\partial x}\right|_{u-\varepsilon}$$

Taking the Laplace transform of both the sides and making use of initial condition given by (2), we get

$$\left.\frac{\partial \hat{\rho}(x,s)}{\partial x}\right|_{u+\varepsilon} - \left.\frac{\partial \hat{\rho}(x,s)}{\partial x}\right|_{u-\varepsilon} = -1 + s\int_{u-\varepsilon}^{u+\varepsilon} dx\hat{\rho}(x,s)$$

Taking the limit $\varepsilon \to 0$ we find

$$\partial_x \hat{\rho}_2\big|_{x=u+\varepsilon} - \partial_x \hat{\rho}_1\big|_{x=u-\varepsilon} = -1. \tag{10}$$

To find the discontinuity in the value of ρ (x,t) across $x = u$, we can first integrate both sides of eq. (5) from 0 to x and then further integrate over x from $u - \varepsilon$ to $u + \varepsilon$, use the property of step function and take the Laplace transform. This will give in the limit $\varepsilon \to 0$,

$$\hat{\rho}(u+\varepsilon,s)\exp A = \hat{\rho}(u-\varepsilon,s), \tag{11}$$

Using eqs. (9), (10), (11) we get the values of the constants C_1, C_2 given by

$$C_1 = \left[\sqrt{s}\left[(\exp(-A))\cosh(\sqrt{s}u) + \sinh(\sqrt{s}u)\right]\right]^{-1}, \tag{12a}$$

$$C_2 = (\exp(\sqrt{s}u - A))\cosh(\sqrt{s}u)C_1. \tag{12b}$$

This completes the solution of the probability distribution function and is in agreement with the one given by Berdichevsky and Gitterman [2].

We have shown that the use of step function in the one dimensional Fokher-Planck equation makes it much simpler to find its complete solution. Since one could introduce step functions in multi dimensional problems also, we feel that the present way of looking at the problem will also be useful when one is dealing with multi dimensional problems.

We have not calculated or discussed the mean square value of x as it has already been discussed in great detail in Ref. [2].

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